Anisotropic electron g-factor in quantum dots with spin-orbit interaction

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g-factor tuning of electrons in quantum dots is studied as function of in-plane and perpendicular magnetic fields for different confinements. Rashba and Dresselhaus effects are considered, and comparison is made between wide- and narrow-gap materials. The interplay between magnetic fields and intrinsic spin-orbit coupling is analyzed, with two distinct phases found in the spectrum for GaAs in perpendicular field. The anisotropy of the g-factor is reported, and good agreement with available experimental findings is obtained.

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Spin properties in semiconductor quantum dots (QDs) have become a field of intense research because of the possible use of the electron spin degree of freedom as a quantum bit.¹ It is then essential to have a clear understanding of the processes that may induce spin relaxation on electrons in the QD; long spin relaxation times, and as pure as possible spin states, are required so that spin can indeed transport information without losses. Insights on the purity of the spin degree of freedom of electrons in QDs can also be extracted from measurements of their effective g-factor.

Manipulation of g-factor in semiconductors and description of its tensorial nature have been considered theoretically as well as experimentally. Among various techniques, appropriate system design has achieved gate-voltage control of g-factor of electrons in a quantum well² and spin manipulation using gigahertz electric fields.³ g-factor measurements have been reported in QDs by means of capacitance⁴ and energy^{5,6} spectroscopies, for example. The tensorial nature of electron q-factor in spherical QDs,⁷ as well as surface⁸ and spatial confinement⁹ effects, where spin-orbit (SO) coupling plays an important role, have been addressed theoretically. We have recently reported on the influence of SO coupling on the electronic spectrum of 2D parabolic QDs. 10 Spin-orbit effects on g-factor have been addressed for 2D electrons in a quantum well¹¹ and for electrons in a parabolic QD,¹² with emphasis on the difference between narrow- and wide-gap compounds.

One of the main causes of spin relaxation and g-factor variation is the SO interaction. When QDs are built in semiconductors of zincblende structure in the plane of a 2D system, there are two possible forms of SO coupling, namely the Rashba¹³ and Dresselhaus¹⁴ interactions; the former is due to the surface inversion asymmetry (SIA) induced by the 2D confinement, while the latter is caused by the bulk inversion asymmetry (BIA) intrinsic in zincblende structures. The SO coupling mixes spins with different orientations in the Zeeman sublevels, which yields an intrinsic spin relaxation source and produces variations in the QD g-factor from the pure Zeeman splitting expected in a magnetic field.

In this work we study the anisotropy of effective g-

factors in 2D parabolic QDs, and analyze the intricate competition¹⁵ between external magnetic fields and intrinsic SO couplings. Wide- and narrow-gap materials with different confinement potentials are considered under in-plane and perpendicular magnetic fields. We show that the q-factor can be tuned to have positive, zero, and negative values at given perpendicular fields, and find that two distinct phases can be present in the QD spectrum, where at low (high) fields the SO coupling enhances (suppresses) the Zeeman sublevel splitting. We find that the widely used perturbative approach 16 based on a unitary transformation¹⁷ of the SO Hamiltonian has strict limitations in QDs if the well defining the 2D confinement has small width. We also show that even for in-plane magnetic fields – typically assumed to yield the bulk g-factor without orbital contributions – the SO coupling reduces the value of g, especially for large QDs.

The QD is defined by an in-plane parabolic confinement, $V(\rho) = m\omega_0^2 \rho^2/2$, where $m(\omega_0)$ is the electronic effective mass (confinement frequency), while the perpendicular confinement V(z) is assumed strong enough to reduce the electronic states to the first conduction subband of the quantum well; its function is $\varphi(z) =$ $\sqrt{2/z_0}\sin(\pi z/z_0)$, z_0 being the QD vertical width for hard wall potential. In the absence of SO interactions, the QD Hamiltonian is $H_0 = \hbar^2 \mathbf{k}^2 / 2m + V(\rho) +$ $g_0\mu_B \mathbf{B}_{\perp} \cdot \sigma/2$, where $\mathbf{k} = -i\nabla + e\mathbf{A}/(\hbar c)$ is the canonical momentum, g_0 is the material bulk g-factor, σ stands for the Pauli matrices, μ_B is the Bohr magneton, and $\mathbf{A} = B_{\perp} \rho(-\sin\phi,\cos\phi,0)/2$ describes a perpendicular magnetic field $\mathbf{B}_{\perp} = B_{\perp}(0,0,1)$, which lifts both orbital and spin degeneracies of levels. H_0 yields the Fock-Darwin (FD) spectrum, ¹⁸ $E_{nl\sigma_z} = (2n + |l| +$ $1)\hbar\Omega + l\hbar\omega_c/2 + g_0\mu_B B_{\perp}\sigma_z/2$, with effective (cyclotron) frequency $\Omega = \sqrt{\omega_0^2 + \omega_c^2/4}$ ($\omega_c = eB_{\perp}/mc$), where n=0,1,2,... and $l=0,\pm 1,\pm 2,...$ are respectively the radial and azimuthal quantum numbers. The FD eigenfunctions are $\Psi_{nl}(x,\phi) = R_{n|l|}(x)e^{il\phi}/\sqrt{2\pi}$, where $R_{n|l|}(x) = \sqrt{2n!/(n+|l|)!}/\lambda x^{|l|}e^{-x^2/2}L_n^{|l|}(x^2)$, in terms of associated Laguerre polynomials $L_n^{|l|}$, $\lambda = \sqrt{\hbar/(m\Omega)}$ is the effective QD lateral length, and $x = \rho/\lambda$.

The SO Hamiltonian added to H_0 is $H_{SO} = H_{SIA} +$

 $H_{BIA}.$ The SIA term, due to the full confining potential $V(\mathbf{r})=V(\rho)+V(z)$ and with coupling parameter $\alpha,$ is given by $H_{SIA}=\alpha\sigma\cdot\nabla V(\mathbf{r})\times\mathbf{k}.$ It can be separated as $H_{SIA}=H_R+H_{LAT},$ where $H_R=-\alpha/\lambda(dV/dz)[\sigma_+L_-A_-+\sigma_-L_+A_+]$ is the Rashba term 13 caused by the interfacial electric field generated by the perpendicular confinement, and $H_{LAT}=\alpha(\hbar\omega_0/l_0^2)\sigma_z[L_z+(\lambda/l_B)^2x^2/2]$ is due to the lateral confinement (diagonal in the FD basis); we define $L_\pm=e^{\pm i\phi},~\sigma_\pm=(\sigma_x\pm i\sigma_y)/2,~L_z=-i\partial/\partial\phi,~$ and $A_\pm=\mp\partial/\partial x+L_z/x+(\lambda/l_B)^2x/2,~$ and the confining (magnetic) length is $l_0=\sqrt{\hbar/(m\omega_0)}$ ($l_B=\sqrt{\hbar/(m\omega_c)}$). The z-confinement yields the BIA term, 14 $H_{BIA}=\gamma[\sigma_xk_x\left(k_y^2-k_z^2\right)+\sigma_yk_y\left(k_z^2-k_x^2\right)+\sigma_zk_z\left(k_x^2-k_y^2\right)]\equiv H_D^L+H_D^C;$ the linear contribution is $H_D^L=-i\gamma\langle k_z^2\rangle/\lambda\left[\sigma_+L_+A_+-\sigma_-L_-A_-\right],~$ while the cubic is $H_D^C=i\gamma/\lambda^3[\sigma_-L_+^3H_1+\sigma_+L_-^3H_2+\sigma_-L_-H_3+\sigma_+L_+H_4],~$ where $H_i=A_i+(\lambda/l_B)^2B_i+(\lambda/l_B)^4C_i+(\lambda/l_B)^6D_i,~$ with i=1,2,3,4. The sixteen functions A_i,B_i,C_i,D_i are known, 10 γ is the coupling parameter, and $\langle k_z^2\rangle=(\pi/z_0)^2$ for hard wall confinement. The total QD Hamiltonian, $H=H_0+H_{LAT}+H_R+H_D^L+H_D^C,$ is diagonalized in a basis set including 110 FD states.

When considering an *in-plane* field (B_{\parallel}) we take the full Hamiltonian above at zero B_{\perp} -field, $H(B_{\perp}=0)$, plus the Zeeman contribution $g_0\mu_B \mathbf{B}_{\parallel} \cdot \sigma/2$, which lifts only the spin degeneracy of levels.

Before discussing the QD effective g-factor, we comment on the influence of SO coupling on the spectrum and its competition with external magnetic fields. This is done in Figs. 1 and 2 respectively for $InSb^{19}$ and $GaAs^{20}$ QDs, the former having larger SO coupling and Zeeman splitting than the latter. In these two figures, left (right) panels refer to an in-plane (perpendicular) field, and dotted lines in panels A and B refer to the pure FD spectrum (no SO-coupling). In panels A and B of Fig. 1, the main effects of the SO interaction on the InSb QD levels are as follows: crossings between FD levels are converted into anticrossings (ACs) according to the selection rules¹⁰ of H_{SO} (and shifted to higher field values in the perpendicular case); the low-field spectrum is displaced to lower energies, while at high-field is not altered much; zero-field splittings appear in the spectrum, and the original FD energy shells are separated into components according to the total angular momentum projection, $j = l + \sigma_z/2$. Panels C and D (E and F) of Fig. 1 show the fieldevolution of spin $\langle \sigma_z \rangle$ (orbital $\langle l \rangle$) angular momentum expectation values for the seven lowest QD levels, where it is clearly visible how the SO coupling mixes states, resulting in σ_z and l no longer reflecting pure FD levels, especially around AC points. For the purposes of discussion, we still label states by the numbers $\{l, \sigma_z\}$ even under SO interaction.

By comparing left (right) panels in Fig. 1, one can obtain the QD level sequence and realize which SO mechanism is responsible for the level ACs under B_{\parallel} (B_{\perp}). Focusing on the lowest energy levels, notice at $B_{\parallel} \simeq 0.1~{\rm T}$

FIG. 1: InSb QD spectrum [19]. Left (right) panels refer to in-plane (perpendicular) magnetic field. Panels A and B show spectra (dotted lines refer to QD without SO interaction). Panels C and D (E and F) show field-evolution of spin (orbital) angular momentum expectation values for the seven lowest levels; ground state is spin-up. Labels in C and D show which SO term is responsible for the lowest ACs. Colors indicate different levels: black, red, green, ... stand for ground, first excited, second excited, ... states, in all panels. A sudden change in line color indicates a level crossing.

FIG. 2: Level spectrum for GaAs QD [20]. B_{\perp} -scale of panel B is different from panels D and F. No AC occurs under B_{\parallel} . Ground state at low B_{\perp} -fields is spin-down, and it is flipped back to spin-up around 13.7 T, as shown in panel D.

that the lowest two states in the first shell have |j| = 1/2 $(\{l, \sigma_z\} = \{0, 1\}, \{0, -1\});$ in the second shell, the two lower states have |j| = 1/2 ($\{-1, 1\}, \{1, -1\}$), while the two upper ones have $|j| = 3/2 \ (\{1,1\}, \{-1,-1\})$. At $B_{\perp} \simeq 0.1$ T, the only difference in such sequence is in the ordering of the two upper states in the second shell, which become |j| = 3/2 ($\{-1, -1\}, \{1, 1\}$). This ordering reversal is due to the influence of B_{\perp} on the orbital features of the state, which changes the effect of SO coupling on these levels; similar features appear in higher shell states. Even though the ground state does not exhibit AC for any field-direction, it is also not spin-pure at low magnetic fields; observe that $\langle \sigma_z \rangle \simeq 0.75$ in both B_{\perp} and B_{\parallel} , and it is positive since g_0 is negative. Regarding level ACs, the lowest under B_{\parallel} ($\simeq 4.8$ T) involves the second and fourth QD states in panel A, which at that field are the levels $\{0, -1\}$ and $\{1, 1\}$; such levels are connected by the operators $\sigma_{\pm}L_{\pm}$, and although they appear in both H_D^C and H_D^L terms, this AC is mostly due to the linear Dresselhaus term as indicated in panel C. On the other hand, the lowest AC under B_{\perp} ($\simeq 3.3$ T) involves the second and third QD states in panel B, which at that field are the levels $\{0, -1\}$ and $\{-1, 1\}$; such levels are connected by the operators $\sigma_{\pm}L_{\mp}$, so that this AC is due to the Rashba term H_R , as indicated in panel D. Higher energy ACs are evident at similar values of B_{\parallel} (or B_{\perp}) and are due to the same SO mechanism. The different SO terms in H, as well as the level dispersion in the two field-configurations producing the ACs, result also in different spin mixings. This clearly affects the QD effective q-factor, as we will see below. ACs due to the cubic Dresselhaus term are also observed at higher fields: at $B_{\perp} \simeq 6$ T the lowest AC involves the fourth and fifth levels, $\{0, -1\}$ and $\{-3, 1\}$, connected by the operators $\sigma_{\mp}L_{\pm}^{3}$. Interestingly, at $B_{\parallel}\simeq 14$ T, where ACs due to H_D^C involve higher energy levels, $\langle l \rangle$ for all QD levels collapse to zero, indicating strong orbital mixing with full spin polarization.

Figure 2 has the same analysis for a GaAs QD. The left panels show that in an in-plane field the SO coupling is not strong enough to induce ACs in the spectrum

(panel A), even though zero-field splittings are clearly observed for different |j| values (e.g., look at the second shell). Notice that levels present the same ordering as in the low- B_{\parallel} InSb QD, and that spin mixing is present in the spectrum, as states do not have $\langle \sigma_z \rangle = \pm 1$ (panel C); e.g., the ground state has $\langle \sigma_z \rangle \simeq 0.75$ at small fields. This shows the intricate interplay between external fields and SO coupling in the definition of electronic properties of QDs. 15 In a perpendicular field (right panels of Fig. 2), however, a new feature is observed: the SO interaction flips the spins of the two lowest levels at low fields, so that the QD ground state becomes a spin-down level. For this reason, the lowest AC at $B_{\perp} \simeq 2$ T (notice different B_{\perp} -scale in panel B compared to D and F) involving the second and third levels, $\{0,1\}$ and $\{-1,-1\}$, is due to the $linear\ Dresselhaus\ term.$ Observe in panel D that those two lowest levels have the same value of $\langle \sigma_z \rangle \simeq -1$ between 4 and 8 T, and that the ground state flips back to its expected spin-up character of a $q_0 < 0$ QD around 13.7 T, when a level crossing is verified in the spectrum (not shown). This result prompts one to consider two distinct ways of defining the QD effective g-factor, and points out strict limits for the validity of the widely used perturbative approach¹⁶ (or unitary transformation¹⁷) for dealing with SO effects in QDs, especially if the well thickness z_0 defining the z-confinement²¹ is small. One has to keep in mind that these results depend on the QD energy (length) scales: higher $E_0 = \hbar \omega_0$ (smaller l_0) QDs are expected to have weaker SO effects, since their level spacing becomes larger.

What is the 'correct' way of defining the effective electron q-factor in a QD? There are two possible definitions involving the two lowest Zeeman sublevels for each field-direction, namely, $g_{\perp,\parallel}^E/g_0 = \Delta E/(g_0 \mu_B B_{\perp,\parallel})$ or $g_{\perp,\parallel}^{\sigma_z}/g_0 = \langle \Delta \sigma_z \rangle/2$, where $\Delta E (\langle \Delta \sigma_z \rangle)$ is the energy splitting (spin expectation value difference) of those levels under $B_{\perp,\parallel}$. Although the first definition is used operationally in experiments where ΔE is measured, the latter is intuitively reasonable since the q-factor is a quantity intrinsically related to the spin value of those levels. For no SO interaction, both definitions yield $g_{\perp} = g_{\parallel} = g_0$, so that no anisotropy is present in the gfactor (other than the material anisotropies).^{2,4} Figures 3 (InSb) and 4 (GaAs) present the g-factor for different QD lateral sizes l_0 , with left (right) panel for in-plane (perpendicular) fields, and dotted lines show results without SO coupling. Panels A and B (C and D) use the definition of g in terms of $\langle \Delta \sigma_z \rangle$ (ΔE), whose values can be inferred from panels C and D of Figs. 1 and 2 (panels Eand F of Figs. 3 and 4). Notice that for InSb in Fig. 3 both definitions yield basically the same *low-field* results for the B_{\parallel} case (panels A and C). The drop in g_{\parallel} is faster in the g^{σ_z} curves because the two lowest states have the same spin at higher fields, while ΔE reaches a constant value (panel E); dotted lines show the field value where the original FD lowest crossing is converted into an AC by the SO coupling at a given E_0 .

In the low-field B_{\perp} case (panels B and D), however,

FIG. 3: Electron g-factor of InSb QDs with different confinement energies E_0 (or lateral sizes l_0). Left (right) panels refer to in-plane (perpendicular) field. Panels A and C (B and D) show g_{\parallel} (g_{\perp}), while panels E and E show sublevel splitting ΔE for the two lowest QD states. Panels E and E (E and E and E (E and E show E as obtained from the E and E calculation; values of E for the 15 meV QD are obtained from Fig. 1. Dotted lines in all panels refer to corresponding QDs without SO coupling. E in panel E is multiplied by 2. Color legend is shown in panel E; dotted lines follow same scheme.

FIG. 4: Same as Fig. 3 but for GaAs QDs. $g_{\perp}^{\sigma_z}$ has inverted sign at low fields indicating that SO coupling is stronger than the Zeeman splitting ($\langle \Delta \sigma_z \rangle$ of the 1.1 meV QD from Fig. 2). g_{\perp}^E has large values at low fields. Dashed lines connecting panels D and F show fields B_g for which $g_{\perp}^E/g_0=1$, and the SO effect is effectively cancelled. Color legend is in panel A. g in panel D is divided by 10.

the two g-factor definitions yield different values mainly at weaker confinements, although the drop in g_{\perp} is also faster in the g^{σ_z} curves (ΔE values are found in panel F). Observe that for the smallest confinement energy (largest SO effect) of 3.0 meV, a sign change is seen in $g_{\perp}^{\sigma_z}$ around 1 T, which relates to an unusual crossing involving the ground and first excited states (compare with panel B of Fig. 1 where this crossing is absent). In both field-directions, smaller E_0 yields smaller g-factor, which shows that SO coupling provides a channel to manipulate g in QDs under magnetic fields. At the same time, a measurement of effective g under $B_{\perp,\parallel}$ might give information about the values of SO constants since, as discussed in Fig. 1, the lowest AC in the spectrum of QDs in different field-directions is due to a distinct SO mechanism. Notice the clear anisotropy in g^E (panels C and D): the same QD confinement shows $g^E_{\perp} < g^E_{\parallel}$, since the mixing with higher orbitals is stronger for B_{\perp} . If the g^{σ_z} definition is considered (panels A and B), such anisotropy is not as remarkable at low fields, although a sign change is obtained at $E_0 = 3$ meV, only in the $g_{\perp}^{\sigma_z}$ curve. Notice that unlike the case with no SO interaction, even B_{\parallel} reduces the g-factor and this reduction can in fact be strong ($\gtrsim 50 \%$ at $l_0 \simeq 300 \text{ Å}$).

Figure 4 shows that for GaAs both definitions in panels A and C give essentially the same values of g_{\parallel} , where ΔE is shown in panel E. Differences are noticed only at high magnetic fields for the weakest confinements (0.7 and 1.1 meV). Results are totally different for the perpendicular field case. Panel B can be understood by looking at panel D of Fig. 2 (for 1.1 meV), where it can be seen that $g_{\perp}^{\sigma_z}$ has inverted sign at low fields, becomes zero for B_{\perp} between 4 and 8 T, then acquires inverted sign again, and suddenly flips back to its 'normal' behavior at 13.7 T; under even higher fields, $g_{\perp}^{\sigma_z}$ goes to zero since the two lowest level spins are aligned. Panel B also shows that larger E_0 values (thus smaller SO coupling) cancels the field range where $g_{\perp}^{\sigma_z}$ is zero. Notice that the weaker the

confinement the smaller the field where the sign change occurs.

One finds totally different results for g_{\perp}^{E} (panel D, with ΔE shown in panel F), which may even assume values 12 times larger than g_0 for the smallest E_0 at low fields; still at low fields, larger E_0 tend to reduce g_{\perp}^E towards g_0 . At high fields (inset G), g_{\perp}^E goes to zero when the level crossing involving the ground state occurs, and after such field it increases again. For every E_0 there is a magnetic field B_q – indicated by the dashed lines connecting panels D and F – where g_\perp^E goes from higher to smaller values than g_0 . In Panel F, differently from what occurs in panel E (and in panels E and F of Fig. 3), the B_q -field defines two distinct phases in the spectrum for a given E_0 : below (above) B_g the SO coupling increases (decreases) the Zeeman sublevel splitting as compared to the case without SO interaction; one can then say that at $B_{\perp} = B_g$, the SO coupling is cancelled by the magnetic field in the formation of the sublevel splitting. Such result emphasizes the intricate competition between external magnetic field and intrinsic SO coupling in QDs. [Notice that if a broad Gaussian well or a larger z_0 is considered, such phases are not observed.²¹ In GaAs QDs, the anisotropic nature of the q-factor is much more pronounced, despite the small values of the SO constants.

We conclude with an experimental comparison. Ref. [5]

reported Zeeman sublevel splittings in GaAs QD having $E_0=1.1$ meV under in-plane field. They found $\Delta E\simeq 200~\mu\text{eV}$ at 10~T, while the corresponding curve in panel E of our Fig. 4 yields $\Delta E\simeq 180~\mu\text{eV}$. In a linear fit, they found $|g|=0.29\pm 0.01$, and from panel A (panel C) of Fig. 4 one has $|g_{\parallel}^{\sigma_z}|=0.30~(|g_{\parallel}^E|=0.31)$ at B=10~T, while $|g_{\parallel}|=0.30$ is found at B=0 from both definitions.

We have shown how SO coupling is able to tune the electron g-factor in QDs and even change its sign. We have analyzed the interplay between SO and Zeeman splittings on QD spectra and shown which SO term causes the lowest ACs in in-plane and perpendicular fields, as well as in different materials. We have seen that for GaAs QDs under B_{\perp} the ground state has its spin character inverted at low fields if a narrow well confines the system in the z-direction. We have identified phases of B_{\perp} in the spectrum where the SO interaction increases or decreases the Zeeman splitting of the lowest QD levels, and explicitly shown the anisotropic nature of g-factor in QDs. All these features would not have been accessed if a perturbative approach had been used, especially for QDs with large lateral size.

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¹⁹ Parameters for InSb are: m = 0.014 m₀, $g_0 = -51$, $\alpha = 500$ Å², $\gamma = 160$ eVÅ³, $E_0 = \hbar \omega_0 = 15$ meV ($l_0 = 190$ Å), $z_0 = 40$ Å, dV/dz = -0.5 meV/Å.

²⁰ Parameters for GaAs are: $m=0.067~{\rm m_0},~g_0=-0.44,~\alpha=4.4~{\rm \AA}^2,~\gamma=26~{\rm eV \mathring{A}}^3,~E_0=\hbar\omega_0=1.1~{\rm meV}~(l_0=320~{\rm \mathring{A}}),~z_0=40~{\rm \mathring{A}},~dV/dz=-0.5~{\rm meV/\mathring{A}}.$ ²¹ Notice that $\langle k_z^2 \rangle = (\pi/z_0)^2$ for a hard wall confinement. If

Notice that $\langle k_z^2 \rangle = (\pi/z_0)^2$ for a hard wall confinement. If a Gaussian well is considered, for example, one has $\langle k_z^2 \rangle = 1/z_0^2$, which yields a linear BIA term a factor of 10 smaller than used in this work, thus decreasing the SO coupling.

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